

FIG. 1

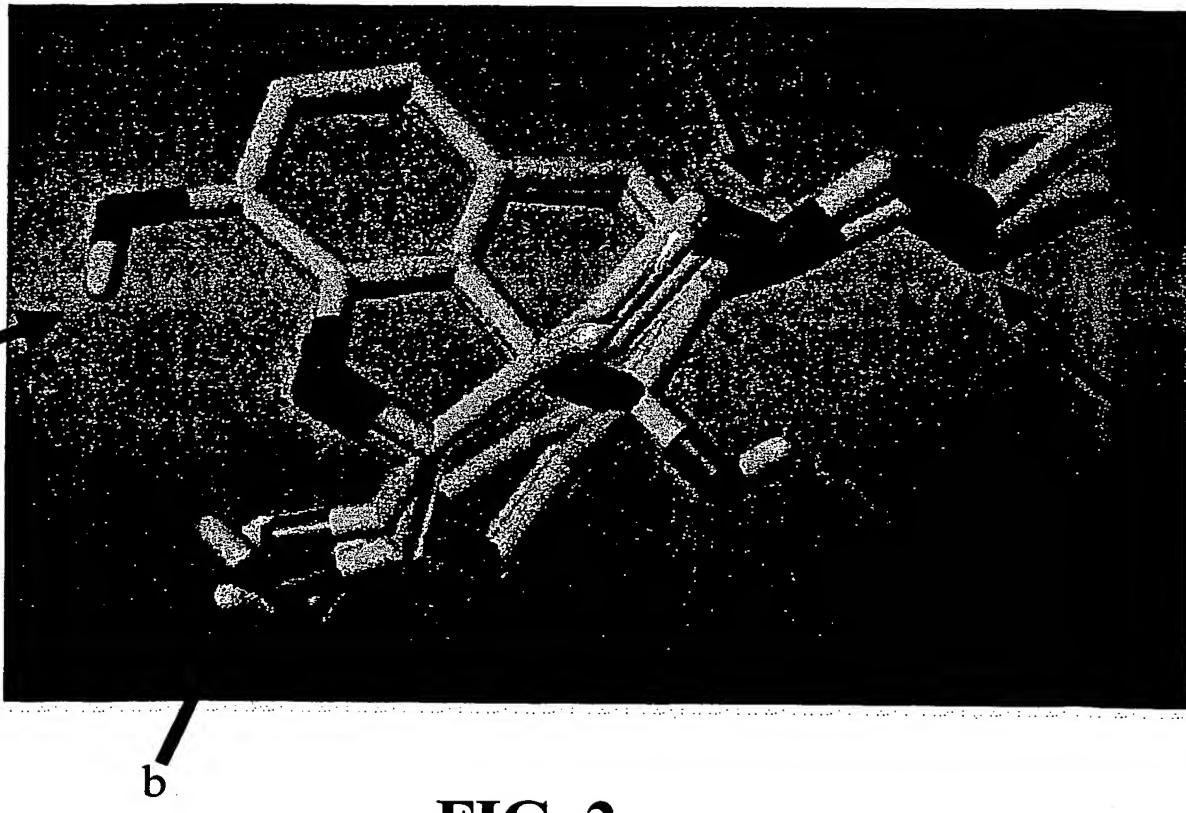


FIG. 2

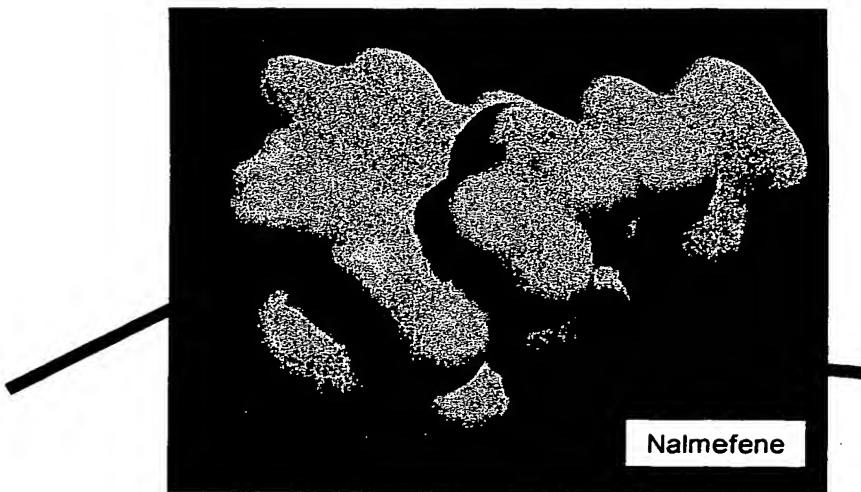


FIG. 3A

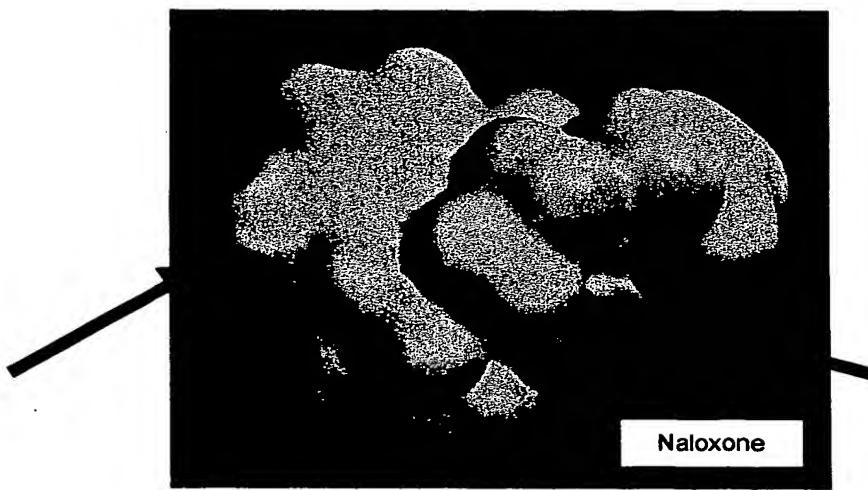


FIG. 3B

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	70413	$C_{19}H_{21}NO_4$	327.384	0.010	Naloxone
	MFCDO0133650	$C_{21}H_{25}NO_3$	339.438	0.018	Nalmefene
	349115	$C_{21}H_{27}NO_3$	341.454	0.406	Nalmefene
	BAS 3387173	$C_{18}H_{21}F_3N_2O_3$	370.375	0.510	Naloxone
	BAS 1002455	$C_{16}H_{19}F_3N_2O_3$	344.337	0.519	Naloxone
	BAS 3387155	$C_{17}H_{19}F_3N_2O_3$	356.348	0.524	Naloxone

Fig. 4A

200 Neighbors

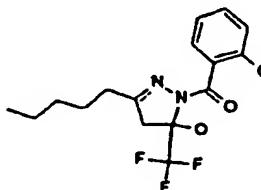
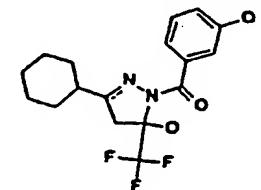
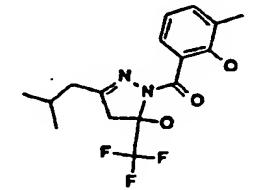
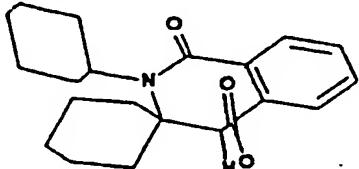
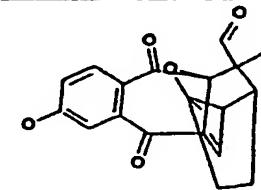
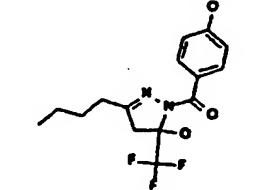
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1268016	$C_{16}H_{19}F_3N_2O_3$	344.337	0.534	Naloxone
	BAS 3387156	$C_{17}H_{19}F_3N_2O_3$	356.348	0.541	Naloxone
	BAS 3387130	$C_{16}H_{19}F_3N_2O_3$	344.337	0.546	Naloxone
	MFCD01935543	$C_{21}H_{27}NO_3$	341.454	0.551	Naloxone
	688277	$C_{20}H_{18}O_5$	338.363	0.591	6-beta-Naloxone
	BAS 1002441	$C_{15}H_{17}F_3N_2O_3$	330.310	0.618	Naloxone

Fig. 4B

200 Neighbors

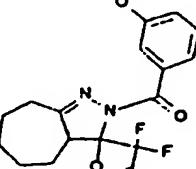
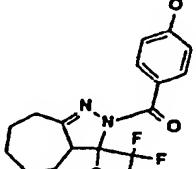
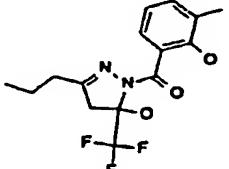
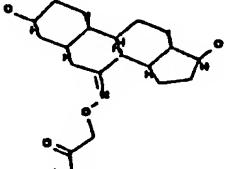
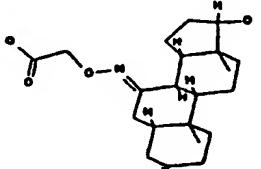
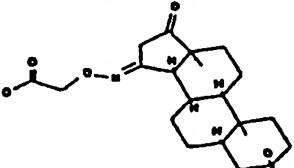
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386059	$C_{16}H_{17}F_3N_2O_3$	342.321	0.637	Naloxone
	BAS 1003176	$C_{16}H_{17}F_3N_2O_3$	342.321	0.637	Naloxone
	BAS 1004848	$C_{15}H_{17}F_3N_2O_3$	330.310	0.643	Naloxone
	MFCD00273259	$C_{21}H_{33}NO_5$	379.501	0.644	Nalmefene
	MFCD00273270	$C_{21}H_{31}NO_5$	377.485	0.646	Naloxone
	MFCD00273266	$C_{21}H_{31}NO_5$	377.485	0.648	Naloxone

Fig. 4C

200 Neighbors

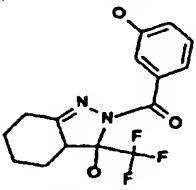
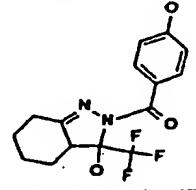
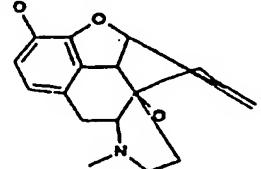
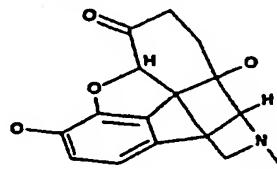
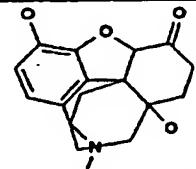
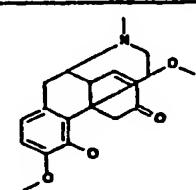
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386023	$C_{15}H_{15}F_3N_2O_3$	328.294	0.653	Naloxone
	BAS 2028128	$C_{15}H_{15}F_3N_2O_3$	328.294	0.657	Naloxone
	617005	$C_{18}H_{21}NO_3$	299.373	0.658	6-beta-Naltrexol
	MFCD00079194	$C_{17}H_{19}NO_4$	301.345	0.682	6-beta-Naltrexol
	19045	$C_{17}H_{19}NO_4$	301.345	0.666	6-beta-Naltrexol
	76021	$C_{19}H_{23}NO_4$	329.399	0.673	Nalmefene

Fig. 4D

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1002442	$C_{15}H_{17}F_3N_2O_3$	330.310	0.677	Naloxone
	MFCD00271723	$C_{23}H_{37}NO_5$	407.555	0.682	Naloxone
	MFCD00273273	$C_{21}H_{29}NO_5$	375.469	0.688	Naimefene
	MFCD00273264	$C_{21}H_{33}NO_5$	379.501	0.697	Naimefene
	BAS 2026145	$C_{16}H_{17}F_3N_2O_3$	342.321	0.698	Naloxone
	BAS 3387114	$C_{15}H_{17}F_3N_2O_3$	330.310	0.704	Naloxone

Fig. 4E

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	376679	$C_{17}H_{18}N_2O_3$	298.345	0.705	Naltrexone
	379963	$C_{17}H_{18}N_2O_3$	298.345	0.705	Naltrexone
	157870	$C_{20}H_{27}NO_4$	345.442	0.714	Nalmefene
	MFCDO0273274	$C_{21}H_{27}NO_5$	373.453	0.720	Naloxone
	MFCDO0273260	$C_{21}H_{33}NO_5$	379.501	0.723	Nalmefene
	BAS 1003163	$C_{16}H_{17}F_3N_2O_3$	342.321	0.727	Naloxone

Fig. 4F

200 Neighbors

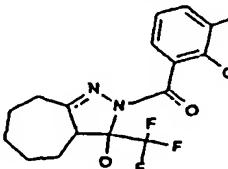
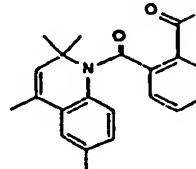
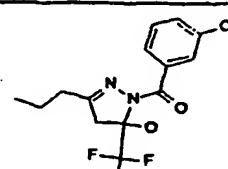
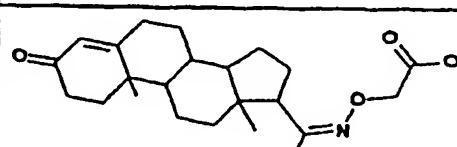
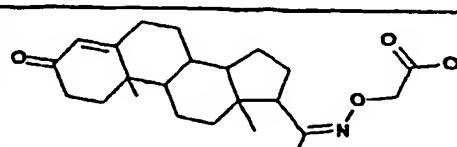
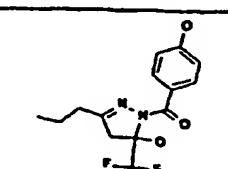
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003182	$C_{17}H_{19}F_3N_2O_3$	356.348	0.739	Naltrexone
	BAS 0510629	$C_{21}H_{21}NO_3$	335.406	0.756	Naltrexone
	BAS 1002419	$C_{14}H_{15}F_3N_2O_3$	316.282	0.757	Naloxone
	18579	$C_{23}H_{33}NO_4$	387.524	0.760	Nalmefene
	58796	$C_{23}H_{33}NO_4$	387.524	0.760	Nalmefene
	BAS 1004835	$C_{14}H_{15}F_3N_2O_3$	316.282	0.763	Naloxone

Fig. 4G

200 Neighbors

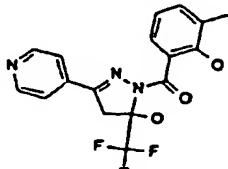
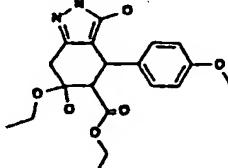
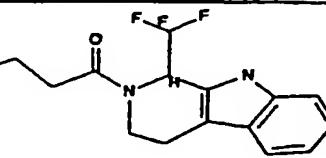
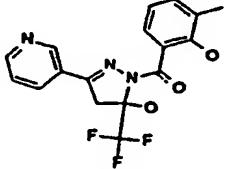
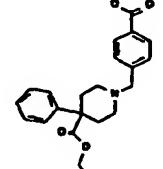
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 2004373	$C_{17}H_{14}F_3N_3O_3$	365.315	0.765	Naloxone
	693856	$C_{19}H_{24}N_2O_6$	376.413	0.768	Nalmefene
	MFCD01784789	$C_{17}H_{17}F_3N_2O_3$	354.332	0.769	Naloxone
	MFCD00271738	$C_{23}H_{37}NO_4$	391.558	0.772	Nalmefene
	BAS 2025996	$C_{17}H_{14}F_3N_3O_3$	365.315	0.774	Naloxone
	BAS 2282169	$C_{22}H_{25}NO_4$	367.449	0.780	Nalmefane

Fig. 4H

200 Neighbors

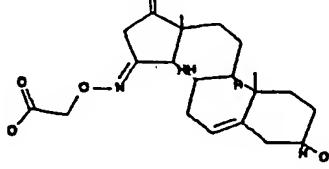
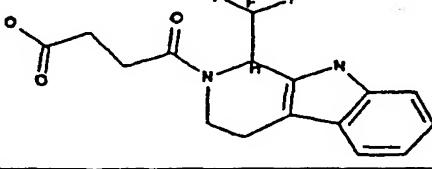
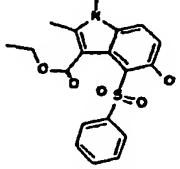
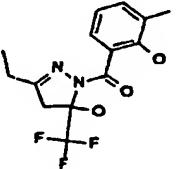
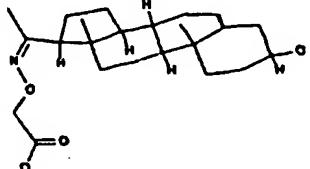
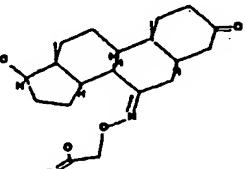
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00273268	C ₂₁ H ₂₉ NO ₅	375.469	0.789	Naloxone
	MFCD00179880	C ₁₆ H ₁₅ F ₃ N ₂ O ₃	340.305	0.800	Naloxone
	BAS 1507170	C ₁₉ H ₁₉ NO ₅ S	373.431	0.801	Nalmefene
	BAS 3386088	C ₁₄ H ₁₅ F ₃ N ₂ O ₃	316.282	0.802	Naloxon
	MFCD00272082	C ₂₃ H ₃₅ NO ₄	389.540	0.818	Nalmefene
	MFCD00271113	C ₂₁ H ₃₁ NO ₅	377.485	0.829	6-beta-Naloxone

Fig. 4I

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	116054	$C_{18}H_{18}N_3O_4$	341.370	0.831	6-beta-Naloxone
	BAS 1004837	$C_{14}H_{15}F_3N_2O_3$	316.282	0.835	Naloxone
	134536	$C_{19}H_{25}NO_3$	315.416	0.836	6-beta-Naloxone
	615801	$C_{17}H_{20}N_2O_3$	300.361	0.856	Naltrexone
	404374	$C_{20}H_{27}NO_3$	329.443	0.870	Nalmefene
	MFCD00273318	$C_{23}H_{35}NO_4$	389.540	0.870	Nalmefene

Fig. 4J

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271094	$C_{21}H_{31}NO_4$	361.486	0.877	Naloxone
	202587	$C_{20}H_{16}O_6$	352.347	0.889	Naloxone
	693862	$C_{18}H_{20}N_2O_6$	360.370	0.892	Naloxone
	MFCD00467140	$C_{19}H_{21}NO_4$	327.384	0.905	Naloxone
	693863	$C_{19}H_{22}N_2O_7$	390.396	0.909	Naltrexone
	MFCD00271196	$C_{21}H_{33}NO_4$	363.501	0.912	Naloxone

Fig. 4K

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386092	$C_{13}H_{13}F_3N_2O_3$	302.255	0.919	Naloxone
	693855	$C_{18}H_{22}N_2O_5$	346.386	0.923	Nalmefene
	BAS 3386091	$C_{13}H_{13}F_3N_2O_3$	302.255	0.928	Naloxone
	MFCD00665833	$C_{16}H_{18}N_2O_2$	270.334	0.929	Naltrexone
	404368	$C_{19}H_{25}NO_3$	315.416	0.941	6-beta-Naltri xol
	BAS 0606820	$C_{13}H_{13}F_3N_2O_4$	318.255	0.948	Naloxone

Fig. 4L

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	693859	$C_{18}H_{22}N_2O_6$	362.388	0.949	Naloxene
	BAS 0436353	$C_{13}H_{13}F_3N_2O_3$	302.255	0.965	Naloxone
	MFCD00167445	$C_{20}H_{20}N_2O_3$	336.394	0.968	Naltrexone
	MFCD00667402	$C_{21}H_{25}NO_6$	387.437	0.974	Naloxene
	MFCD02258126	$C_{18}H_{25}NO_6$	351.403	0.977	Naloxone
	MFCD00143186	$C_{19}H_{21}NO_5$	343.383	0.985	Naltrexone

Fig. 4M

200 Neighbors

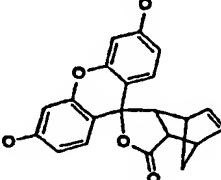
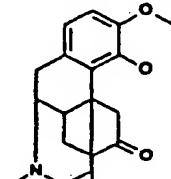
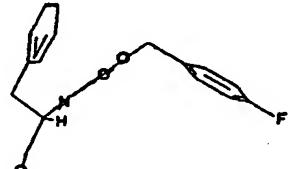
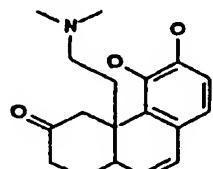
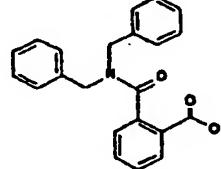
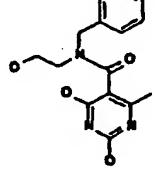
Structure	Cpd ID		MW	Distance	Neighbor
	119887	$C_{21}H_{16}O_5$	348.359	0.993	Naloxone
	404365	$C_{19}H_{25}NO_3$	315.416	1.002	Nalmefene
	MFCD01871411	$C_{21}H_{20}FNO_3$	353.397	1.012	Naloxone
	152720	$C_{18}H_{23}NO_3$	301.389	1.015	6-beta-Naloxol
	117581	$C_{22}H_{19}NO_3$	345.402	1.016	Naloxone
	669466	$C_{15}H_{17}N_3O_4$	303.320	1.017	Naloxone

Fig. 4N

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271129	$C_{21}H_{33}NO_4$	363.501	1.029	Nalmefene
	689431	$C_{20}H_{26}N_2O_3$	342.442	1.035	6-beta-Naloxone
	MFCD00056772	$C_{19}H_{21}NO_3$	311.384	1.039	Nalmefene
	MFCD00199295	$C_{20}H_{27}NO_3$	329.443	1.045	Nalmefene
	R191469	$C_{20}H_{27}NO_3$	329.443	1.046	Nalmefene
	375504	$C_{23}H_{27}NO_5$	397.475	1.050	Naloxone

Fig. 4O

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	692397	$C_{17}H_{13}NO_4$	295.297	1.068	Naloxone
	MFCD00433684	$C_{15}H_{15}NO_3$	257.292	1.069	Naloxone
	693860	$C_{20}H_{24}N_2O_6$	388.424	1.071	Nalmefene
	MFCD01764791	$C_{16}H_{15}F_3N_2O_4$	356.304	1.073	Naloxone
	BAS 1519270	$C_{22}H_{19}NO_3$	345.402	1.078	Naloxone
	BAS 3385849	$C_{12}H_{11}F_3N_2O_3$	288.228	1.083	Naloxone

Fig. 4P

200 Nighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00673308	$C_{21}H_{32}N_2O_2$	344.501	1.087	Naloxone
	404356	$C_{18}H_{21}NO_3$	299.373	1.099	Naloxone
	43938	$C_{22}H_{19}NO_4$	361.401	1.107	Naloxone
	117181	$C_{20}H_{20}N_2O_3$	336.394	1.109	Naltrexone
	MFCD00094379	$C_{24}H_{22}O_2$	342.442	1.111	Naloxone
	404369	$C_{19}H_{25}NO_3$	315.416	1.111	6-beta-Naloxanol

Fig. 4Q

200 Neighbors

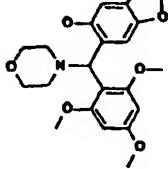
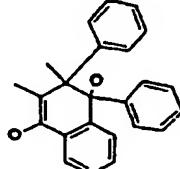
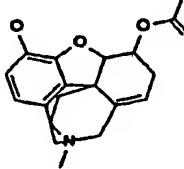
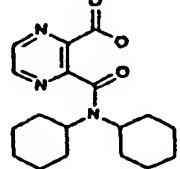
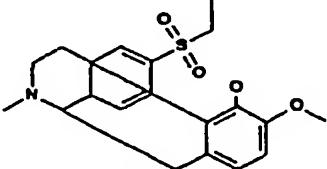
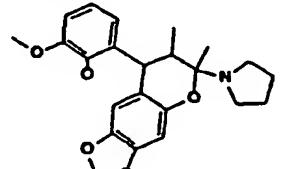
Structure	Cpd ID		MW	Distance	Neighbor
	381577	$C_{21}H_{25}NO_7$	403.436	1.111	Naloxone
	S842214	$C_{24}H_{22}O_2$	342.442	1.112	Nalmefene
	134602	$C_{19}H_{21}NO_4$	327.384	1.112	S-beta-Naloxenol
	CHS 0316796	$C_{18}H_{25}N_3O_3$	331.418	1.113	Naloxone
	134604	$C_{20}H_{25}NO_4S$	375.491	1.115	Nalmefene
	R171697	$C_{23}H_{27}NO_5$	397.475	1.133	Nalmefene

Fig. 4R

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00667401	$C_{23}H_{27}NO_5$	397.475	1.134	Naloxene
	S959863	$C_{18}H_{24}ClNO_3$	337.850	1.137	6-beta-Naloxane
	35545	$C_{18}H_{23}NO_3$	301.389	1.137	6-alpha-Naloxane
	134598	$C_{18}H_{23}NO_3$	301.389	1.137	6-beta-Naloxane
	S310778	$C_{18}H_{14}O_3$	278.310	1.140	Naloxone
	669800	$C_{17}H_{23}NO_2$	273.378	1.141	Naloxone

Fig. 4S

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 0083962	$C_{23}H_{27}N_5O$	389.505	1.141	Naltrexone
	MFCD01765597	$C_{18}H_{21}N_3O_2$	311.387	1.142	6-beta-Naltrexol
	682334	$C_{21}H_{15}FO_3$	334.350	1.143	Naloxone
	BAS 0631739	$C_{18}H_{19}N_3O$	293.372	1.143	Nalmefene
	MFCD00144882	$C_{18}H_{21}NO_3$	299.373	1.149	6-beta-Naltrexol
	MFCD00229975	$C_{18}H_{14}O_3$	278.310	1.150	Naloxone

Fig. 4T

200 N lghbors

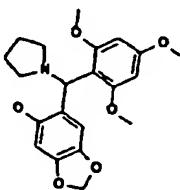
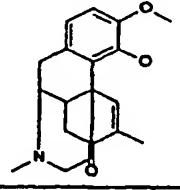
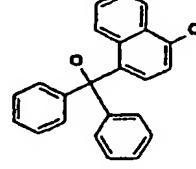
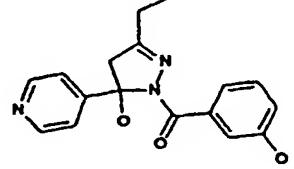
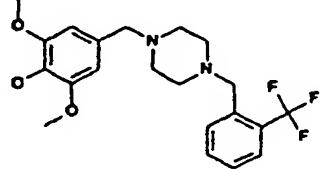
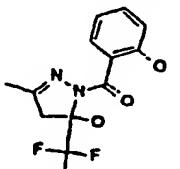
Structure	Cpd ID		MW	Distance	Neighbor
	R171700	$C_{21}H_{25}NO_6$	387.437	1.157	Nalmefene
	134592	$C_{19}H_{23}NO_3$	313.400	1.163	6-beta-Naloxone
	401210	$C_{23}H_{18}O_2$	326.399	1.166	Nalmefene
	BAS 2026074	$C_{17}H_{17}N_3O_3$	311.343	1.172	Naltrexone
	BAS 3050727	$C_{21}H_{25}F_3N_2O_3$	410.440	1.177	Nalmefene
	BAS 0341630	$C_{12}H_{11}F_3N_2O_3$	288.228	1.185	Naloxone

Fig. 4U

200 Neighbors

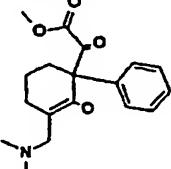
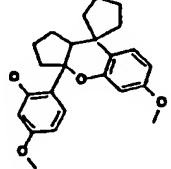
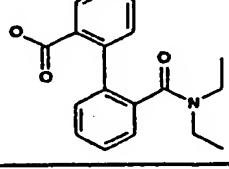
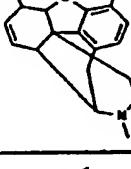
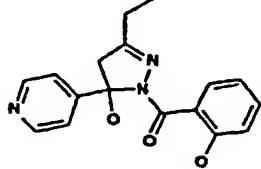
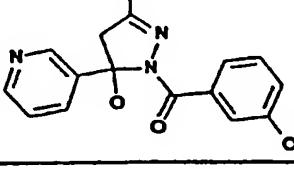
Structure	Cpd ID		MW	Distance	Neighbor
	97817	$C_{18}H_{23}NO_4$	317.388	1.190	Naloxone
	ASN 3185453	$C_{24}H_{28}O_4$	380.488	1.196	Naloxone
	21257	$C_{18}H_{19}NO_3$	297.357	1.196	6-beta-Naltrexol
	134601	$C_{18}H_{21}NO_3$	299.373	1.200	6-beta-Naltrazol
	BAS 2026075	$C_{17}H_{17}N_3O_3$	311.343	1.203	6-beta-Naltrazol
	BAS 1996620	$C_{16}H_{15}N_3O_3$	297.316	1.211	6-beta-Naltrazol

Fig. 4V

200 Neighbors

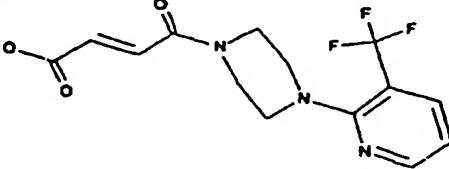
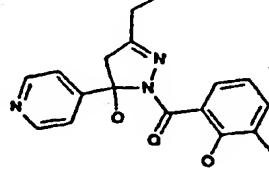
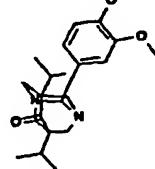
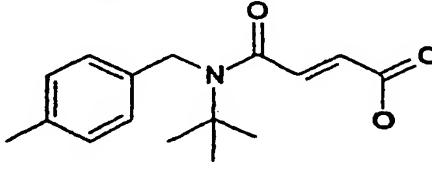
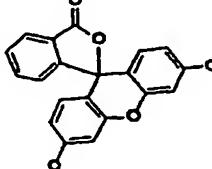
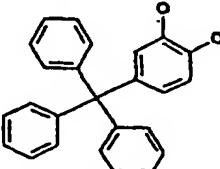
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD01314358	$C_{14}H_{14}F_3N_3O_3$	329.281	1.215	Naloxone
	BAS 2026097	$C_{18}H_{19}N_3O_3$	325.370	1.221	Naloxone
	BAS 1914007	$C_{21}H_{30}N_2O_3$	358.485	1.221	Naloxone
	CHS 0003221	$C_{16}H_{21}NO_3$	275.351	1.227	Naloxone
	667256	$C_{20}H_{12}O_5$	332.316	1.227	Naloxone
	37625	$C_{25}H_{20}O_2$	352.437	1.235	Nalmefene

Fig. 4W

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003093	C ₁₆ H ₁₅ N ₃ O ₃	297.316	1.238	6-beta-Naloxetanol
	16468	C ₂₀ H ₁₄ O ₄	318.332	1.238	Naloxone
	CHS 0227049	C ₁₈ H ₂₃ NO ₃	301.389	1.241	Naloxone
	BAS 0315050	C ₂₂ H ₂₄ N ₄ O ₂	376.462	1.241	Nalmefene
	BAS 1289763	C ₁₈ H ₂₃ NO ₃	301.389	1.242	Naloxone
	349127	C ₁₇ H ₁₉ NO ₄	301.345	1.243	Naloxone

Fig. 4X

200 Neighbors

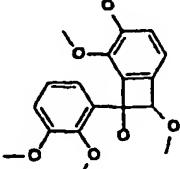
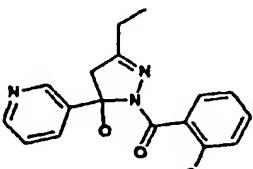
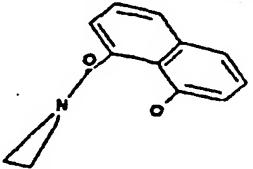
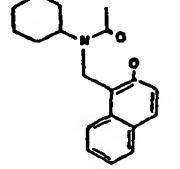
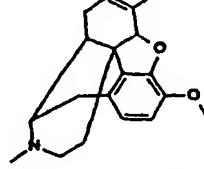
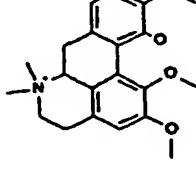
Structure	Cpd ID		MW	Distance	Neighbor
	635928	$C_{18}H_{20}O_6$	332.356	1.250	Nalmefene
	BAS 2377555	$C_{17}H_{17}N_3O_3$	311.343	1.251	6-beta-Naloxane
	MFCD00665835	$C_{15}H_{15}NO_2$	241.292	1.251	Naloxone
	47931	$C_{19}H_{23}NO_2$	297.401	1.255	6-beta-Naloxane
	76435	$C_{18}H_{21}NO_3$	299.373	1.257	Nalmefene
	90558	$C_{21}H_{26}NO_4$	358.446	1.258	Naloxone

Fig. 4Y

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00206273	$C_{20}H_{21}N_3O_2$	335.409	1.261	Naloxone
	159208	$C_{17}H_{19}NO_4$	301.345	1.267	Nalmefene
	BAS 0341580	$C_{16}H_{13}ClN_2O_3$	316.747	1.267	Naltrexone
	BAS 2377575	$C_{18}H_{19}N_3O_3$	325.370	1.268	Naltrexone
	MFCD01765638	$C_{19}H_{17}N_3O_2$	319.366	1.268	Nalmefene
	R171484	$C_{20}H_{23}NO_5$	357.410	1.268	Nalmefene

Fig. 4Z

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighb r
	700350	$C_{15}H_{23}N_5O_2$	305.383	1.272	Naloxone
	16907	$C_{20}H_{15}NO_4$	333.347	1.274	Nalmefene
	R170623	$C_{21}H_{25}NO_5$	371.437	1.275	Nalmefene
	S98907	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	10464	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	215214	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone

Fig. 4AA

200 Neighbors

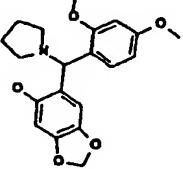
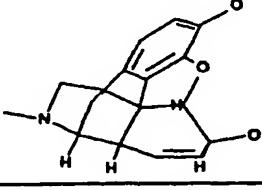
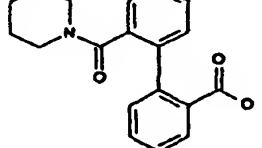
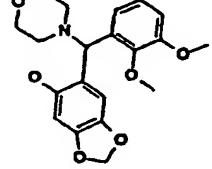
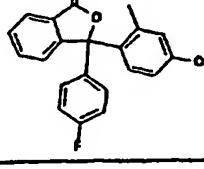
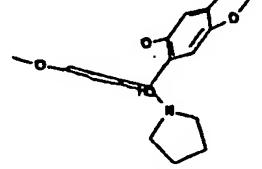
Structure	Cpd ID		MW	Distance	Neighbor
	R171425	C ₂₀ H ₂₃ NO ₅	357.410	1.280	Nalmefene
	MFCD00153032	C ₁₇ H ₁₉ NO ₃	285.346	1.283	6-beta-Naltrexol
	S196991	C ₁₉ H ₁₉ NO ₃	309.368	1.285	Naltrexone
	R170291	C ₂₀ H ₂₃ NO ₈	373.409	1.286	Naloxone
	682335	C ₂₁ H ₁₅ FO ₃	334.350	1.287	Naloxone
	MFCD00667377	C ₂₀ H ₂₃ NO ₅	357.410	1.289	Nalmefene

Fig. 4AB

200 Neighbors

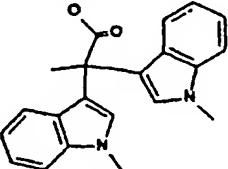
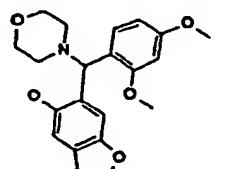
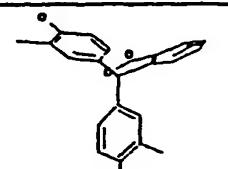
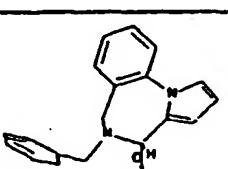
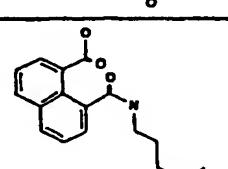
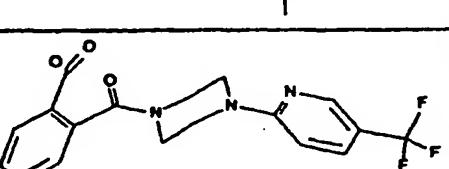
Structure	Cpd ID		MW	Distance	Neighbor
	106242	$C_{21}H_{20}N_2O_2$	332.406	1.294	Naloxone
	R170410	$C_{20}H_{23}NO_6$	373.409	1.299	Naloxone
	MFCD00005912	$C_{22}H_{18}O_4$	346.386	1.300	Naloxone
	MFCD01765637	$C_{20}H_{18}N_2O_2$	318.379	1.302	Nalmefene
	376678	$C_{17}H_{20}N_2O_3$	300.361	1.303	Naltrexone
	MFCD01314431	$C_{18}H_{16}F_3N_3O_3$	379.342	1.303	Naloxone

Fig. 4AC

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	370278	$C_{21}H_{25}NO_5$	371.437	1.304	Naloxone
	MFCD00242635	$C_{17}H_{19}NO_3$	285.346	1.305	6-beta-Naltrexol
	S602965	$C_{15}H_{15}NO_3$	257.292	1.306	Naltrexone
	370279	$C_{20}H_{23}NO_5$	357.410	1.306	Naloxone
	157877	$C_{18}H_{25}NO_3$	303.405	1.310	Naloxone
	19046	$C_{17}H_{19}NO_3$	285.346	1.310	6-beta-Naltrexol

Fig. 4AD

200 Neighbors

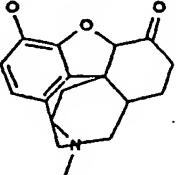
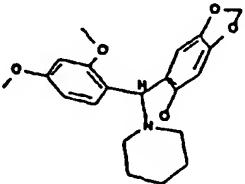
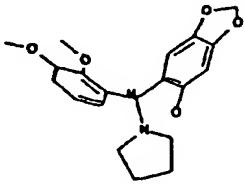
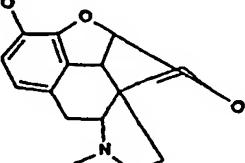
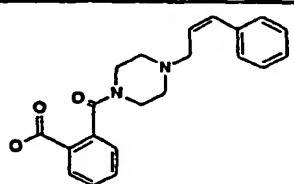
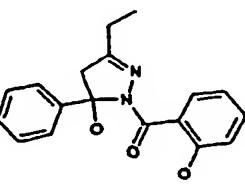
Structure	Cpd ID		MW	Distance	Neighbor
	117862	$C_{17}H_{19}NO_3$	285.346	1.310	6-beta-Naltr exol
	MFCD00667305	$C_{21}H_{25}NO_5$	371.437	1.313	Nalmefene
	MFCD00667382	$C_{20}H_{23}NO_5$	357.410	1.316	Nalmefene
	611276	$C_{17}H_{19}NO_3$	285.346	1.318	6-beta-Naltr exol
	BAS 1099232	$C_{21}H_{22}N_2O_3$	350.421	1.320	Naltrexone
	BAS 0313319	$C_{18}H_{18}N_2O_3$	310.356	1.321	6-beta-Naltr exol

Fig. 4AE

200 Neighbors

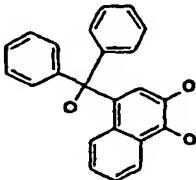
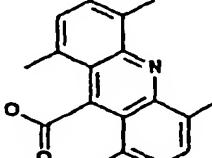
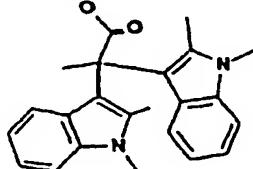
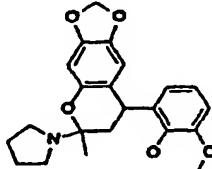
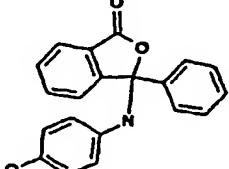
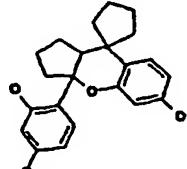
Structure	Cpd ID		MW	Distance	Neighbor
	401211	$C_{23}H_{18}O_3$	342.398	1.325	Naloxene
	409635	$C_{18}H_{17}NO_2$	279.342	1.326	Naloxene
	106231	$C_{23}H_{24}N_2O_2$	360.460	1.327	Naloxone
	375505	$C_{22}H_{25}NO_5$	383.448	1.329	Naloxone
	BAS 1053035	$C_{20}H_{15}NO_3$	317.347	1.331	Naloxone
	ASN 3160807	$C_{22}H_{24}O_4$	352.434	1.332	Naloxone

Fig. 4AF

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	324633	$C_{21}H_{26}O_6$	374.438	1.333	Naloxone
	370277	$C_{20}H_{23}NO_6$	373.409	1.339	Naloxone
	MFCD00375811	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naloxone
	BAS 0659522	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naloxone
	CHS 0305736	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naloxone
	381576	$C_{20}H_{23}NO_6$	373.409	1.348	Naloxone

Fig. 4AG

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	CHS 0120289	$C_{17}H_{15}NO_3$	281.314	1.348	Naloxone
	351159	$C_{23}H_{20}N_2O_2$	356.428	1.349	Nalmefene

Fig. 4AH

http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2633336/figure/F1/

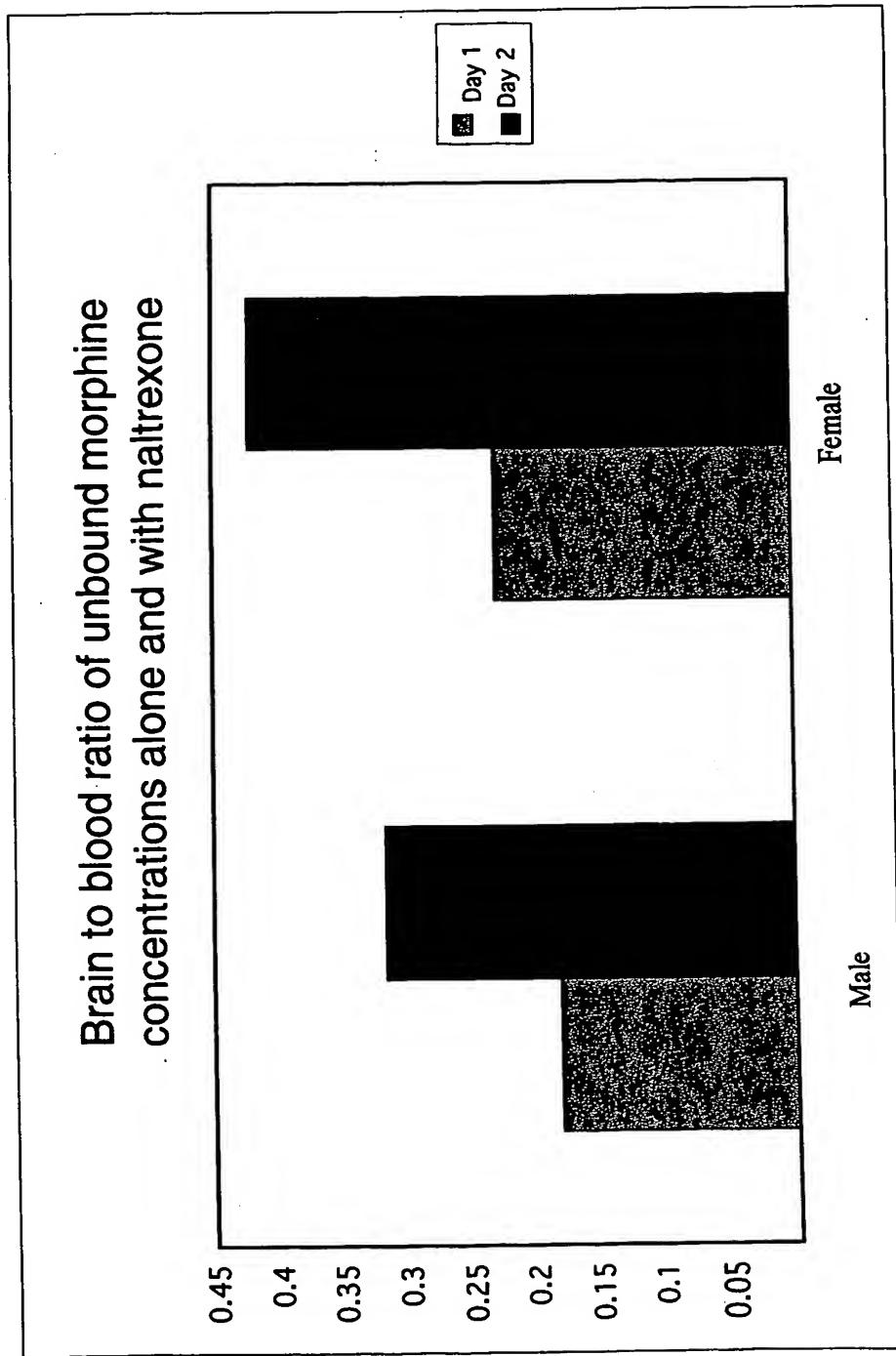
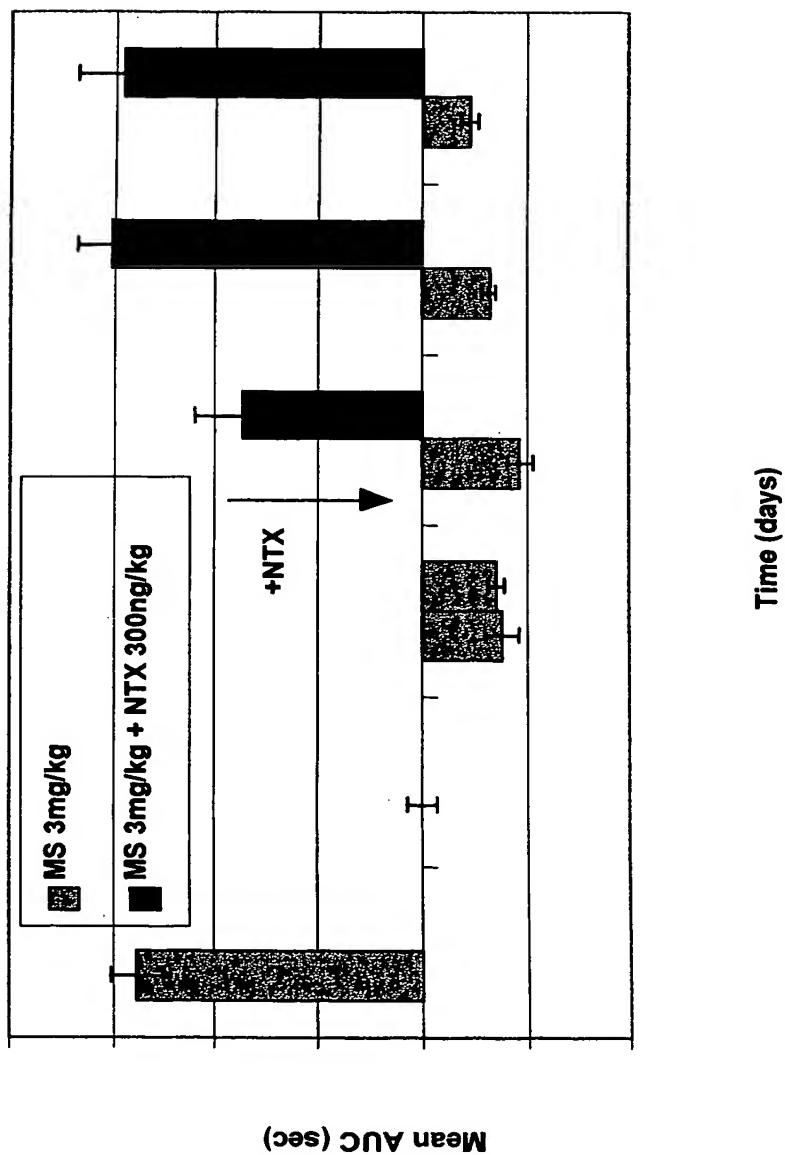


FIG. 5

Fig. 6

MS 3mg/kg
MS 3mg/kg+NTX 3000ng/kg

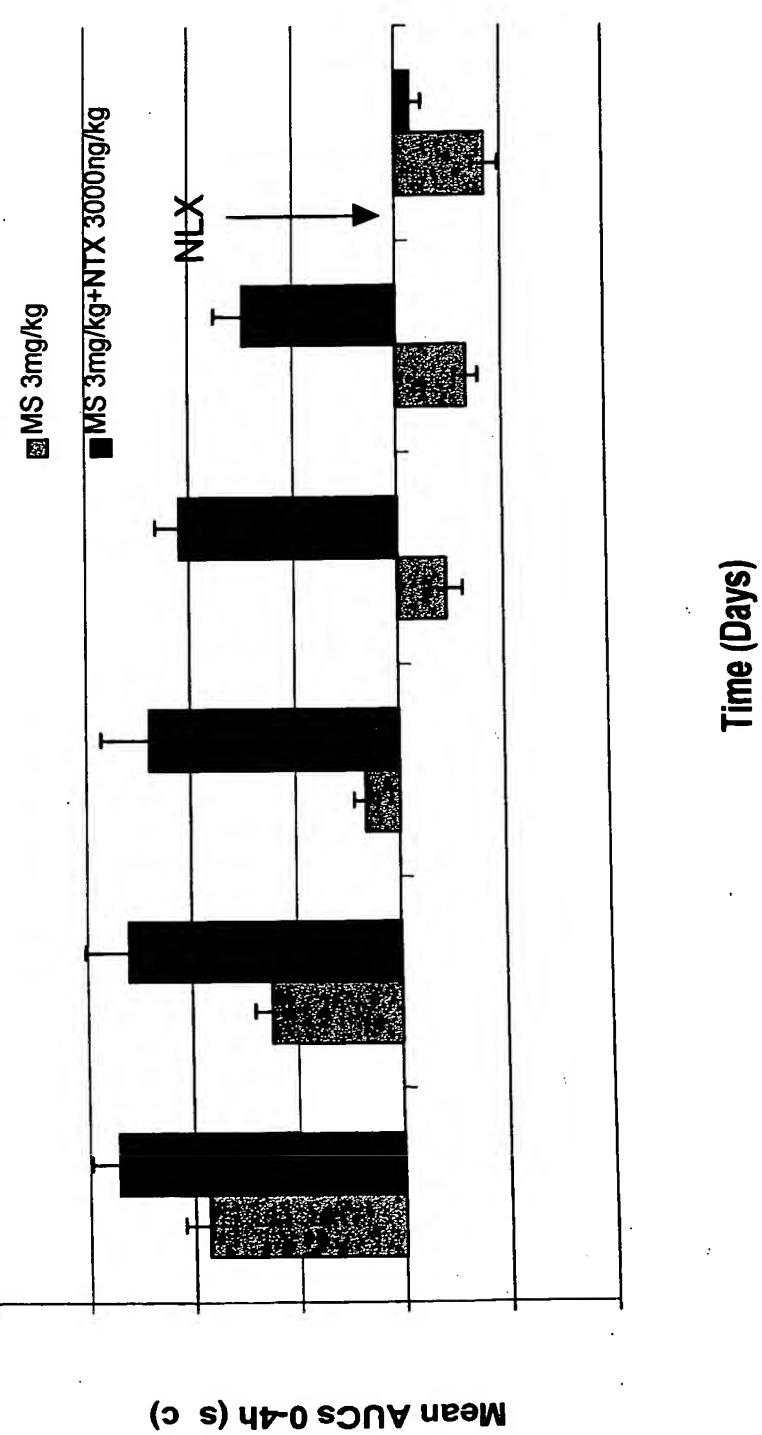


Fig. 7